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THEORY OF HETEROJUNCTION DISCONTINUITIES.(U)
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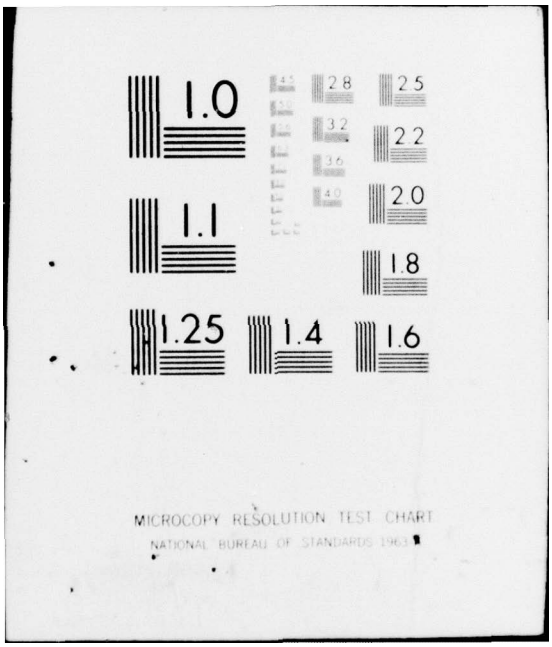
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The findings in this report are not to be construed as an official Department of the Army position, unless so designated by other authorized documents.

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

Heterojunctions
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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

The problem of theoretically understanding and predicting the energy band lineups at abrupt semiconductor heterojunctions was investigated. Methods were developed that represent a significant advance in the problem and that permit a prediction of the band edge discontinuities from the known energy band structures, by means of self-consistent pseudopotential calculations.

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1.) Introduction

This is the Final Report to ARO Grant # DAHCO4-74-G-0114, "Theory of Heterojunction Discontinuities," for the period 1 February 1974 - 30 September 1976. The Principal Investigator was Dr. Herbert Kroemer, during the grant, Professor of Electrical Engineering at the University of Colorado (CU), now in the same capacity at the University of California at Santa Barbara (UCSB). The grant had originally been awarded through 31 January 1977; it was terminated earlier because of Dr. Kroemer's move to UCSB. The work is actually continued at UCSB under a follow-up grant (#DAAG29-77-G-0017).

2.) The Problem

The problem studied was the theoretical understanding of the energy band lineup at semiconductor heterojunctions, and the development of theoretical means to predict that lineup for new and as yet untried heterojunction pairs.

Heterojunctions are junctions between different semiconductors, such as GaAs and AlAs. They are increasingly being employed in advanced semiconductor devices, and the performance of the devices depends on the relative lineup of the energy bands at the junctions. Prior to this work the only rule for the prediction of the lineup was the electron affinity rule. It is theoretically ill-founded, and in practice hard to apply, because it requires empirical surface property data on high-quality crystals. Even where such data are available, the predictions made from them often do not agree with the results obtained on actual

heterojunctions -- once the latter have been prepared, often at great technological expense.

What was desired was a better theoretical understanding of why the heterojunctions line up the way they do, on a level that would make it possible to predict the lineup, with a minimum of technological investment, and thus to aid in making decisions as to whether or not the odds are favorable to make it worthwhile to embark on the possibly very expensive technology to build a particular new device. Very substantial progress was made under this grant towards this goal.

Techniques were developed that permit one to determine the band lineup at abrupt heterojunction pairs, provided only that accurate bulk energy band structures are known for the participating semiconductors. By performing self-consistent pseudopotential calculations in which the theoretical energy bands are matched to the empirical ones, an absolute reference potential can be calculated which governs the band lineup at heterojunctions. In those cases where good actual lineup data were available, the agreement, while not perfect, was so good that there can be little doubt about the soundness of the method.

The method has been applied to new heterojunction pairs, leading to predictions such as the following:

a) At lattice-matched InP-(In,Ga)(As,P) junctions most of the energy gap discontinuity should occur in the valence band.

b) At lattice-matched InAs-Ga(As,Sb) or InAs-Al(As,Sb) heterojunctions the conduction band edge of InAs should

be close to -- or even below -- the valence band edge on the other side.

One of the effects originally thought to be important was found to be essentially non-existent: A dipole moment at the heterojunction interface due to the tunneling of electrons from the higher of the two valence bands into the forbidden gap across the junction.

3.) Publications and Reports

3.1) Publications

1) W.R. Frensley, H.A. Schauer, and H. Kroemer, "Contribution of Dielectric Image Force to the Conduction Band Discontinuity in Semiconductor Heterojunctions," Bull. Am. Phys. Soc. II, Vol. 20, p. 426, March 1975.
2) H. Kroemer, "Problems in the Theory of Heterojunction Discontinuities," CRC Crit. Revs. in Solid State Science, Vol. 5 (#4), pp. 555-564, November 1975.
3) W.R. Frensley, "Prediction of Semiconductor Heterojunction Discontinuities from Bulk Band Structures," J. Vac. Sci. Technol., Vol. 13 (#4), pp. 810-815, July/Aug. 1976.

3.2) Technical Reports

W.R. Frensley, "A Model for the Prediction of Semiconductor Heterojunction Discontinuities using Buld Band Structures," Interim Technical Report, September 1976. This is a verbatim copy of the complete Ph.D. Thesis of Dr. Frensley, and it contains the principal results obtained under this grant.

4.) Participating Scientific Personnel and Advanced Degrees Earned under this Grant

4.1) Principal Investigator: Dr. Herbert Kroemer, Professor of Electrical Engineering

4.2) Graduate Research Assistants:

1.) William R. Frensley, Graduate Student in Physics, received Ph.D. August 1976, with thesis listed as item (3.2) above.

2.) Henry A. Schauer, Graduate Student in Applied Physics, recieved Ph.D. September 1976, with thesis,"The Contribution and Standing Wave Effects within the Valence Band to Heterojunction Discontinuities."

4.3) Undergraduate Students

Mr. Steve Wright, Undergraduate Student in Electrical Engineering, assisted in calculations.